Chemtura Corporation
Benson Road 2-19
Middlebury, CT 06749
Regulatory Compliance

December 21, 2005

Administrator
ATTN: Chemical Right-to-Know Program
US Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116

Dear Sir or Madam:
Re: Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol (CAS No. 116265-68-0)

Chemtura Corporation is providing this letter and submission of a Test Plan and robust summaries as part of our commitment to sponsor CAS Number 116265-68-0 (Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol) under the HPV Challenge Program.

If you have any questions regarding our commitment, please feel free to contact me at (203) 573-2219 or Alan.Taylor@chemtura.com. You may also contact Dr. Wendy Koch, Epona Associates, LLC at (860) 429-0038 or wendykoch@eponallc.com.

Yours very truly,

Alan Taylor
Regulatory Compliance
Chemtura Corporation

Attachments: Test Plan
Appendices 1 and 2

cc Charles M. Auer, Director
Office of Pollution Prevention and Toxics
US EPA Headquarters
1200 Pennsylvania Avenue, N.W.
Mail Code: 7401M
Washington, DC 20460

PHOSPHOROUS ACID, TRIPHENYL ESTER, REACTION PRODUCTS WITH DIPROPYLENE GLYCOL (CAS NO. 116265-68-0): TEST PLAN

Submitted to the US Environmental Protection Agency

By

Chemtura Corporation

DATE: December 21, 2005

SUMMARY

Chemtura Corporation (Chemtura) has sponsored Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0) under the EPA's High Production Volume (HPV) Program. This document provides the Test Plan and summaries of existing data for this substance.

1.0 INTRODUCTION

Chemtura has voluntarily committed to participate in the Environmental Protection Agency's (EPA) high production volume chemicals (HPV) challenge program (program), to assess the health and environmental hazards, including selected physical chemical characteristics of Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol (CAS No. 116265-68-0). This substance is represented by a second CAS No.; 36788-39-3, 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethyl ethoxy)methylethoxy]tetramethyl-. These two CAS No. are the same substance, and data from either substance represents the sponsored substance.

An evaluation of the available data and proposed test plan are included in this document. Robust summaries are attached in Appendix 1.

The objective of this test plan is to evaluate the available data and determine what additional data, if any, are needed to adequately characterize the physical properties, environmental fate, and human health and environmental hazards of Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol (CAS No. 116265-68-0). It is proposed that additional studies be conducted as shown in Table 1.

Table 1: PROPOSED TESTING FOR PHOSPHOROUS ACID, TRIPHENYL ESTER, REACTION PRODUCTS WITH DIPROPYLENE GLYCOL (CAS NO. 116265-68-0)

Endpoint	Data
Physical Chemical Properties	
Melting Point	A
Vapor Pressure	A
Boiling Point	A
Partition Coefficient	A
Water Solubility	Test
Environmental Fate	
Hydrolysis	Test
Photodegradation	A
Biodegradation	Test
Environmental Transport	A
Ecotoxicity	
Acute Fish	Test
Acute Daphnia	Test
Acute Algae	Test
Mammalian toxicity	
Acute Oral	A
Acute Dermal	A
Acute Inhalation	A
Repeated Dose	Test
Genotoxicity (*in vitro* -bacteria)	Test
Genotoxicity (*in vivo*)	Test
Reproductive/Developmental	Test

A= Adequate data
Test = Testing proposed

2.0 POTENTIAL USE AND EXPOSURE

The sponsored substance is one of several related phosphite materials used as a secondary antioxidant in polyolefins, ABS, synthetic rubber, PVC, epoxies, polyurethanes, polyesters, adhesives and other polymers to improve color, processing, heat and UV stability. Some typical applications include polyethylene films, refrigerator liners and vinyl flooring. Materials of this type are also used in lubrication additives.

3.0 EVALUATION OF EXISTING DATA AND PROPOSED TESTING

The available data have been assessed (see Tables 2 through 4). Robust summaries are provided as Appendix 1.

Chemical/Physical Properties:

The vapor pressure of the sponsored substance is 1.3-13.3 hPa (Crompton, 2003). The physical chemical properties of the substance were calculated using EPIWIN (see Appendix 2). Based on calculated data, the sponsored substance is expected to have a high water solubility and low partition coefficient. However, the substance is expected to be insoluble (Crompton, 2003), such that a water solubility test is proposed.

TABLE 2: PHYSICAL CHEMICAL PROPERTIES FOR PHOSPHOROUS ACID, TRIPHENYL ESTER, REACTION PRODUCTS WITH DIPROPYLENE GLYCOL (CAS NO. 116265-68-0)

Endpoint	CAS NO. 116265-68-0
Melting Point	187 C
Vapor Pressure	1.3-13.4 hPa
Boiling Point	484 C
Partition Coefficient	-1.56
Water Solubility	Insoluble

Recommendation: A water solubility test (OECD 105) is proposed.

Environmental Fate:

Environmental fate data are not available for the sponsored substance. EPIWIN was used to predict the photodegradation and environmental distribution (see Appendix 2). The Overall OH Rate Constant = 200.6758 E-12 cm3/molecule-sec and the predicted half-life = 0.053 days. Level III fugacity modeling distribution to water and soil will predominate. Although it is expected that hydrolysis of the sponsored substance will be slow, testing is proposed in order to clarify the hydrolysis rate. Biodegradation of the sponsored substance is not available; a biodegradation study is proposed.

Recommendation: A hydrolysis test (OECD 111) and a biodegradation test (OECD 301) are proposed.

TABLE 3: ENVIRONMENTAL FATE DATA FOR PHOSPHOROUS ACID, TRIPHENYL ESTER, REACTION PRODUCTS WITH DIPROPYLENE GLYCOL (CAS NO. 116265-68-0)

Endpoint	CAS NO. 116265-68-0
Hydrolysis	Slow
Photodegradation	Overall OH Rate Constant = 200.6758 E-12 cm3/molecule-sec Half-Life = 0.053 Days
Biodegradation	Not available
Environmental Transport (Level III Fugacity modeling)	Air $4.36x10^{-10}$ Water 49.8 Soil 50.1 Sediment 0.0918

Recommendation: A hydrolysis test (OECD 111) and biodegradation study (OECD 301) are proposed.

Aquatic Toxicity

Acute aquatic toxicity data are not available for fish, daphnia or algae for the sponsored substance.

Recommendation: Acute aquatic toxicity studies with fish, daphnia and algae (OECD 203, 202, and 201) are proposed.

Acute Mammalian Toxicity

Acute oral, dermal and inhalation studies have been conducted (Crompton, 2003). The data indicate low toxicity by all routes of exposure.

Recommendation: No additional testing is proposed.

Repeated Dose/ Reproductive/Developmental Toxicity

No data are available regarding the repeated dose toxicity, reproductive toxicity or developmental effects of the sponsored substance or structurally related substances.

Recommendation: A combined repeat dose with developmental and reproductive screen (OECD 422) is proposed.

Mutagenicity Assays

No data were located for in vitro or in vivo mutagenicity.

Recommendation: Bacterial (OECD 471) and in vitro mammalian mutagenicity (OECD 473) studies are proposed.

TABLE 4: MAMMALIAN TOXICITY DATA FOR PHOSPHOROUS ACID, TRIPHENYL ESTER, REACTION PRODUCTS WITH DIPROPYLENE GLYCOL (CAS NO. 116265-68-0)

Endpoint	CAS NO. 116265-68-0
Acute Oral	>10,000 mg/kg (rat)
Acute Dermal	>2000 mg/kg (rabbit)
Acute Inhalation	>2 mg/L (rat)
Repeated Dose	Not available
Genotoxicity (*in vitro* - bacteria)	Not available
Genotoxicity (*in vivo*)	Not available
Reproductive/Developmental	Not available

REFERENCES

Crompton (2003) Material Safety Data Sheet, Weston 430. Revision 1.2; 10/15/2003

EPI SUMMARY (v3.11)

APPENDIX 1
ROBUST SUMMARIES

I U C L I D

Data Set

Existing Chemical	:	ID: 116265-68-0
Producer related part		
Company	:	Epona Associates, LLC
Creation date	:	12.12.2005
Substance related part		
Company	:	Epona Associates, LLC
Creation date	:	12.12.2005
Status	:	
Memo	:	Phosphorous acid, triphenyl ester, reaction products with dipropylene glycol
Printing date	:	21.12.2005
Revision date	:	
Date of last update	:	20.12.2005
Number of pages	:	10
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	= 187 °C
Sublimation	:	
Method	:	other: calculated
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41)
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Result	:	Melting Pt (deg C): 187.09 (Mean or Weighted MP)
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Value obtained using modeling
Flag	:	Critical study for SIDS endpoint

20.12.2005 (2)

2.2 BOILING POINT

Value	:	= 484 °C at
Decomposition	:	
Method	:	other: calculated
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41)
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Result	:	Boiling Pt (deg C): 484.31 (Adapted Stein & Brown method)
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Value obtained using modeling
Flag	:	Critical study for SIDS endpoint

20.12.2005 (2)

2.4 VAPOUR PRESSURE

Value	:	= 1.3 - 13.4 hPa at °C
Decomposition	:	
Method	:	other (measured)
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-

hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.

Test substance : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No.: 36788-39-3

Reliability : (2) valid with restrictions
Internal company data

Flag : Critical study for SIDS endpoint

20.12.2005 (1)

Value : = .0000000000017 hPa at 25 °C
Decomposition :
Method : other (calculated)
Year : 2005
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41)
Remark : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Result : VP(mm Hg, 25 deg C): 1.28E-012 (Modified Grain method)
Test substance : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No.: 36788-39-3
Reliability : (3) invalid
Value obtained using modeling is in disagreement with actual data

20.12.2005 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = -1.56 at 25 °C
pH value :
Method : other (calculated)
Year : 2005
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.67 estimate)
Remark : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Result : Log Kow (KOWWIN v1.67 estimate) = -1.56
Test substance : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No.: 36788-39-3
Reliability : (2) valid with restrictions
Value obtained using modeling
Flag : Critical study for SIDS endpoint

20.12.2005 (2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	42610 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Water Solubility Estimate from Log Kow (WSKOW v1.41): Water Solubility at 25 deg C (mg/L): 4.261e+004 log Kow used: -1.56 (estimated) no-melting pt equation used
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Result	:	Water Solubility at 25 deg C (mg/L): 4.261e+004
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Value obtained using modeling
Flag	:	Critical study for SIDS endpoint

20.12.2005 (2)

Solubility in	:	Water
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Result	:	Insoluble
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Internal company data
Flag	:	Critical study for SIDS endpoint

20.12.2005 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	
Conc. of sensitizer	:	
Rate constant	:	= .0000000002 cm^3/(molecule*sec)
Degradation	:	50 % after .1 day(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Atmospheric Oxidation (25 deg C) [AopWin v1.91]
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Result	:	Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 200.6758 E-12 cm3/molecule-sec Half-Life = 0.053 Days (12-hr day; 1.5E6 OH/cm3) Half-Life = 0.640 Hrs Ozone Reaction: No Ozone Reaction Estimation
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Value obtained using modeling
Flag	:	Critical study for SIDS endpoint

20.12.2005 (2)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	other
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Result	:	Hydrolyzes slowly
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions

Internal company data
Flag : Critical study for SIDS endpoint
20.12.2005 (1)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: estimated
Year : 2005

Remark : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.

Result :

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	7.64e-006	1.28	1000
Water	49.8	900	1000
Soil	50.1	900	1000
Sediment	0.0918	3.6e+003	0

Persistence Time: 789 hr

Test substance : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-
CAS No.: 36788-39-3

Reliability : (2) valid with restrictions
Value obtained using modeling

Flag : Critical study for SIDS endpoint
12.12.2005 (2)

3.5 BIODEGRADATION

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 10000 mg/kg bw
Species	:	rat
Strain	:	no data
Sex	:	no data
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Internal company data
Flag	:	Critical study for SIDS endpoint

20.12.2005 (1)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 2 mg/l
Species	:	rat
Strain	:	no data
Sex	:	no data
Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	
Method	:	other
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Internal company data
Flag	:	Critical study for SIDS endpoint

20.12.2005 (1)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 2000 - mg/kg bw
Species	:	rabbit
Strain	:	no data
Sex	:	no data
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	2003
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No: 36788-39-3 is the same as Phosphorous acid, triphenyl ester, reaction products with dipropylene Glycol (CAS No. 116265-68-0.
Test substance	:	3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl- CAS No.: 36788-39-3
Reliability	:	(2) valid with restrictions Internal company data

20.12.2005 (1)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

9. References

(1) Crompton (2003) Material Safety Data Sheet, Weston 430. Revision 1.2; 10/15/2003

(2) EPI SUMMARY (v3.11)

APPENDIX 2
EPIWIN RESULTS

SMILES : OC(COCC(OP(OC(COCC(O)C)C)OCC(OC(CO)C)C)C)C
CHEM : 3,6,8,11-Tetraoxa-7-phosphatridecane-1,13-diol, 7-[2-(2-hydroxymethyl ethoxy)methylethoxy]tetramethyl-
CAS NUM: 036788-39-3
MOL FOR: C18 H39 O9 P1
MOL WT : 430.48

---------- EPI SUMMARY (v3.11) ----------

Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : 9.1
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.67 estimate) = -1.56

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
Boiling Pt (deg C): 484.31 (Adapted Stein & Brown method)
Melting Pt (deg C): 187.09 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 1.28E-012 (Modified Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.41):
Water Solubility at 25 deg C (mg/L): 4.261e+004
log Kow used: -1.56 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 1.1011e+005 mg/L

ECOSAR Class Program (ECOSAR v0.99g):
Class(es) found:
Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:
Bond Method : 2.52E-017 atm-m3/mole
Group Method: Incomplete
Henrys LC [VP/WSol estimate using EPI values]: 1.210E-004 atm-m3/mole

Probability of Rapid Biodegradation (BIOWIN v4.01):
Linear Model : -0.0233
Non-Linear Model : 0.0000
Expert Survey Biodegradation Results:
Ultimate Survey Model: 2.7018 (weeks-months)
Primary Survey Model : 3.5858 (days-weeks)
Readily Biodegradable Probability (MITI Model):
Linear Model : -0.0858
Non-Linear Model : 0.0060

Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 200.6758 E-12 cm3/molecule-sec
Half-Life = 0.053 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 0.640 Hrs
Ozone Reaction:
No Ozone Reaction Estimation

Soil Adsorption Coefficient (PCKOCWIN v1.66):
     Koc   : 10
     Log Koc: 1.000

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:
   Rate constants can NOT be estimated for this structure!

BCF Estimate from Log Kow (BCFWIN v2.15):
   Log BCF = 0.500 (BCF = 3.162)
      log Kow used: -1.56 (estimated)

Volatilization from Water:
   Henry LC: 2.52E-017 atm-m3/mole (estimated by Bond SAR Method)
   Half-Life from Model River: 4.82E+013 hours   (2.009E+012 days)
   Half-Life from Model Lake : 5.259E+014 hours   (2.191E+013 days)

Removal In Wastewater Treatment (recommended maximum 99%):
   Total removal: 1.85 percent
   Total biodegradation: 0.09 percent
   Total sludge adsorption: 1.75 percent
   Total to Air: 0.00 percent

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	4.36e-010	1.28	1000
Water	49.8	900	1000
Soil	50.1	900	1000
Sediment	0.0918	3.6e+003	0

   Persistence Time: 789 hr
